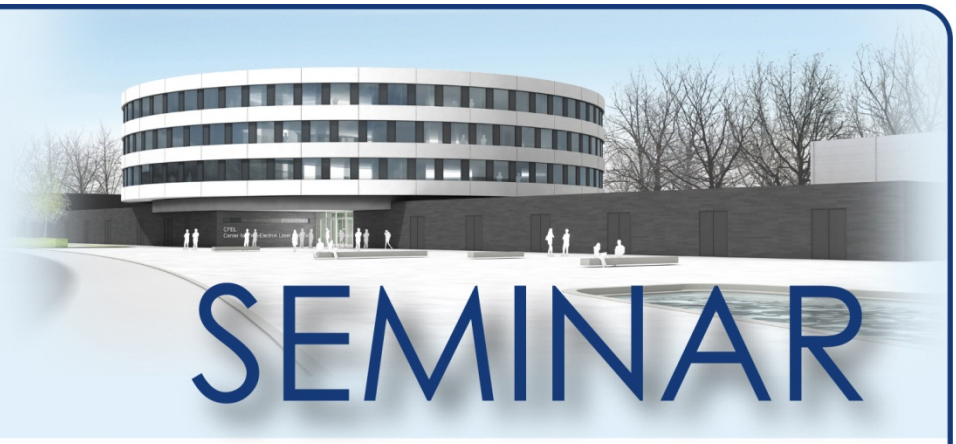
CFEL SCIENCE



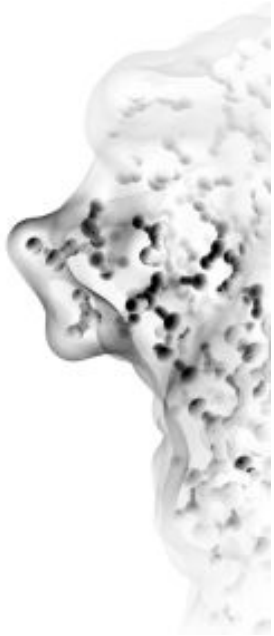
SEMINAR

19th September 2011 - 16:00
Building 49, Seminar Room (108)

Erik Marklund

Uppsala University, Sweden

Gas-phase protein structure under the computational microscope



Although the native environment of the vast majority of proteins is a complex aqueous solution, like the interior of a cell, many analysis methods for assessing chemical and physical properties of biomolecules require the sample to be aerosolized; that is, transferred to the gas-phase. An important example is electrospray-ionization mass spectrometry, which can provide a wide range of information about e.g. biomolecules. That includes structural features, charged sites, and gas-phase equilibrium constants of reactions. To date much of the microscopic detail about the aerosolization process remains beyond the limits of experimental observation. How is the gas-phase structure of a protein related to the solution-phase structure? How transferrable are observations done in the gas phase to solution? On the basis of classical molecular-dynamics simulations important features of gas-phase biomolecular structure near the end of the the aerosolization process are revealed: the relation between gas-phase structure and native structure, microscopic detail about the de-wetting of gas-phase biomolecules, and the impact of temperature and residual solvent on structure preservation. Advances in simulation of proton-transfer reactions further expand the range of scientific problems that can be addressed with molecular dynamics, including studies of gas-phase proteins.

Host: Henry Chapman, CFEL CI Seminar